

magnetic moments. They give origin to a surface contribution to the susceptibility that follows a nearly perfect Curie law and appear to have antiferromagnetic interactions. Our results are in qualitative agreement with the experimental results obtained so far⁴ and the theoretical estimates for the magnetic moment and Néel temperature are close to the experimental values. However, the polycrystalline nature of the samples used in the experiments prevents direct quantitative comparison. It would clearly be very interesting to perform similar experiments on single-crystal surfaces.

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Summary Abstract: Study of temperature and hydrogen induced reconstruction and reordering of W(100) by polarized electron scattering

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An intense polarized electron beam¹ obtained by photoemission from negative electron affinity GaAs(100) was used to scatter electrons from the high temperature W(100) (1×1) phase, ($\sqrt{2} \times \sqrt{2}$) R45° phase at 100 K, and the hydrogen chemisorbed $c(2 \times 2)$ and (1×1) phases in order to study the structure changes due to temperature and to hydrogen chemisorption. This interesting system has been the object of numerous investigations as seen in the recent papers of King and Thomas² and Barker and Estrup.³ It is the purpose of this work to investigate the sensitivity of spin-dependent electron scattering to the structural changes which occur in these four different phases. We can draw qualitative conclusions from our polarized low energy electron diffraction (PLEED) data, and the data provide a basis for further structural analysis when dynamical PLEED calculations of this system become available.

The spin-orbit interaction causes the cross section for electrons with spin aligned parallel, $I_{\uparrow\uparrow}$, or antiparallel, $I_{\uparrow\downarrow}$, to their orbital angular momentum to be different. The strength of the spin dependent scattering, $S(E)$, is defined as $(1/P_0)[I_{\uparrow\uparrow}(E) - I_{\uparrow\downarrow}(E)]/[I_{\uparrow\uparrow}(E) + I_{\uparrow\downarrow}(E)]$, where $1/P_0$ makes S independent of the degree of polarization of the incident beam, and $I(E) = (1/2)(I_{\uparrow\uparrow} + I_{\uparrow\downarrow})$ is the spin averaged LEED intensity observed in conventional LEED experiment. S has been shown to be sensitive to adsorbates.⁴ For light adsorbates, a significant new term in the spin dependent scattering comes from the interference between the spin-orbit

scattering of the substrate atoms and the Coulomb scattering of the adsorbate. The relative adsorbate position with respect to the substrate atoms is contained in this interference term and may provide chemical bonding information. In the case of H adsorption discussed in this work, the adsorbate Coulomb scattering is very small; therefore, changes in S on H adsorption are due to reconstruction of the substrate giving a different substrate-Coulomb and substrate spin-orbit scattering interference.

The details of the polarized electron source, the LEED apparatus, and the data acquisition have been described elsewhere.^{1,5} The crystal used was mechanically polished to within $\frac{1}{4}^\circ$ of the W(100) plane. Angular profiles of the intensity of one of the (11) beams at various incident electron energies were measured. The FWHM's showed no obvious oscillatory behavior as a function of energy and were compatible with the FWHM's of the primary beam implying a good surface with large terrace width which is consistent with a $\frac{1}{4}^\circ$ uncertainty of the (100) orientation. The crystal can be flashed to 2500 K for cleaning and can be cooled to 100 K within about 20 min. The total pressure remained at about 4×10^{-11} Torr (5×10^{-9} Pa) during the experiment. Hydrogen was admitted in the PLEED chamber through a UHV valve at a partial pressure of 1×10^{-9} Torr (1.3×10^{-7} Pa).

The quantities $S(E)$ and $I(E)$ were measured for the (00) specular beam at angles of incidence from 10° to 21° in an [010] azimuth and at normal incidence for the (0 $\bar{1}$), (0 $\bar{2}$), (1 $\bar{1}$),

(22), $(\bar{1}/2, \bar{1}/2)$ and $(3/2, \bar{3}/2)$ nonspecular beams. There are many differences found in the $S(E)$ profiles from the different phases of W even where the differences in LEED intensity profiles, $I(E)$, are small as will be reported in a complete paper elsewhere.⁶ The effect on the (01) beam, for example, of lowering the temperature of clean W(100) is to change the magnitude of S at $140 < E < 180$ eV while the I profiles are about the same. The changes in magnitude and sign in the S profiles from all the nonspecular beams implies that the lateral positions of the W atoms are changed; this is consistent with the previously suggested lateral displacement model.^{2,3}

The effect of hydrogen chemisorption at a coverage $\theta = 0.1$ and at saturation $\theta = 1$ causes dramatic changes in S for the (01) beam as compared to the $(\sqrt{2} \times \sqrt{2}) R45^\circ$ phase in the energy range $70 < E < 100$ eV. The S profile at saturation hydrogen coverage where a (1×1) pattern is observed does not all resemble the S profile for clean W(100). The large differences in S for the $(\sqrt{2} \times \sqrt{2}) R45^\circ$ and $C(2 \times 2)$ -H phases indicates that hydrogen does not just stabilize the low temperature phase but induces a different structure. This is consistent with there being two different structures, such as the displacive structures proposed by King and Thomas² and observed recently by Barker and Estrup.³

The intrinsic properties of the $S(E)$ profiles, e.g., sharp

structure, and sign changes, amplify the subtle difference observed in $I(E)$ profiles and show up as significant differences in $S(E)$ profiles. Also the fact that $S(E)$ is to first order independent of the instrument response function⁷ makes the profile extremely reproducible and directly comparable to a PLEED dynamical calculation without any deconvolution of the measured S . Thus, PLEED provides significant additional information for the determination of the structure of the different phases of W.

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